A NEW METHOD FOR THE STRUCTURE ANALYSIS OF NON-CENTRO-SYMMETRIC CRYSTALS

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NO direct methods are available at present for the determination of the phases of structure factors of a single non-centrosymmetric crystal. If two isomorphous crystals are available and if the positions of the replaceable atoms (A) in the unit cell can be fixed, then the phases of the various reflections can be determined but for an ambiguity between two possible values. This ambiguity is in the sign of the phase θ with respect to the phase of the contribution from the replaceable atom, say, $\alpha_A(hkl)$, so that the phase of the structure factor $F(hkl)$ may be either $\alpha_1 = \alpha_A + \theta$ or $\alpha_2 = \alpha_A - \theta$. In all the determinations made so far, the replaceable atoms are related by a centre of inversion so that the phase $\alpha_A(hkl)$ is either 0 or π and so $\alpha_1 = -\alpha_2$. In such a case, if a Fourier synthesis is calculated using both α_1 and α_2, then the resulting diagram will consist of the structure, duplicated by its inverse at the inversion-centre of the replaceable atoms.. If the replaceable atoms do not have a centre of symmetry, then no simple relation exists between the Fourier synthesis calculated by using both α_1 and α_2 and the actual structure.

DETERMINATION OF PHASE FROM ANOMALOUS DISPERSION

It is possible to obtain the phases directly, without the need for an isomorphous pair of crystals by making use of effects of anomalous dispersion. Suppose the crystal contains one atom or a set of atoms, for which the imaginary component of the scattering factor is appreciable, while for all the other atoms, this component is negligible. Such a situation occurs in a large number of organic compounds, containing a halogen or sulphur or a metal atom, in addition to C, N and O. In such a case, it is possible to find the phase $\alpha(hkl)$ with reference to the phase $\alpha_A(hkl)$ of the anomalous scatterer.

Fig. 1 represents the various components of the structure amplitudes of a reflection hkl and its inverse $\bar{h}\,\bar{k}\,\bar{l}$. The latter are indicated by a bar over the symbols. F_A' is that part of the contribution from the anomalous scatterer which depends upon normal dispersion and F_A''

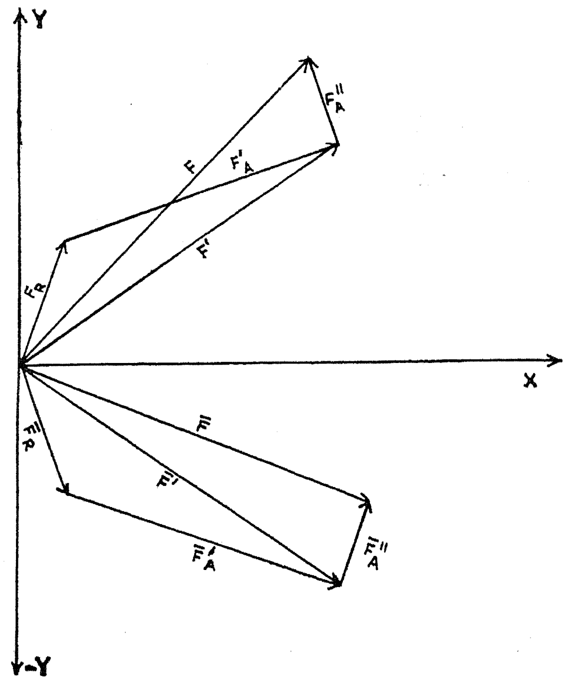
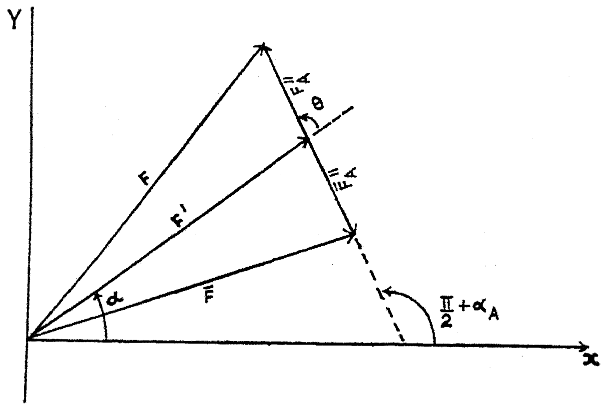


FIG. 1. Diagram showing the relationship between the various components of the structure amplitudes of reflections hkl and $\bar{h}\,\bar{k}\,\bar{l}$.

is the part which is produced by anomalous dispersion and F_R is the net contribution from all the other non-anomalous scatterers. The relationship between F, F' and F_A'' is particularly brought out in Fig. 2 where the vectors



(a)

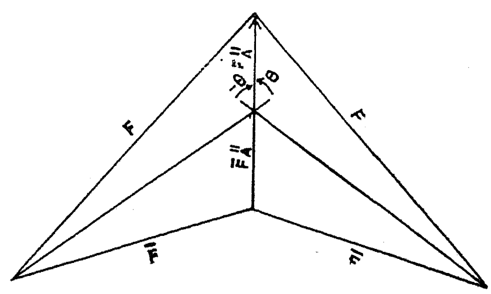


FIG. 2. Relation between F, $\bar{F}$ and F_A'' (b)